

CRYSTAL FRAMEWORKS, MATRIX-VALUED FUNCTIONS AND RIGIDITY OPERATORS

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ABSTRACT. An introduction and survey is given of some recent work on the infinitesimal dynamics of *crystal frameworks*, that is, of translationally periodic discrete bond-node structures in \mathbb{R}^d , for $d = 2, 3, \dots$. We discuss the rigidity matrix, a fundamental object from finite bar-joint framework theory, rigidity operators, matrix-function representations and low energy phonons. These phonons in material crystals, such as quartz and zeolites, are known as rigid unit modes, or RUMs, and are associated with the relative motions of rigid units, such as SiO_4 tetrahedra in the tetrahedral polyhedral bond-node model for quartz. We also introduce semi-infinite crystal frameworks, bi-crystal frameworks and associated multi-variable Toeplitz operators.

1. INTRODUCTION

A survey is given of some recent work on the infinitesimal dynamics of *crystal frameworks*, by which we mean translationally periodic discrete bar-joint frameworks in \mathbb{R}^d . This includes a discussion of rigidity operators, matrix symbol function representations and the connections with models for low energy phonon modes in various material crystals. These modes are also known as rigid unit modes, or RUMs, reflecting their origin in the relative motion of rigid units in the crystalline structure. I also introduce briefly the contexts of semi-infinite crystal frameworks and bicrystal frameworks and indicate how their rigidity operators involve multivariable Toeplitz operators whose symbol functions are matrices over multi-variable trigonometric polynomials on the d -torus.

The topic of infinite bar-joint frameworks, whether periodic or not, can be pursued as a purely mathematical endeavour and many aspects of deformability and rigidity remain to be understood. The main perspectives below and related issues are developed in Owen and Power [22], [23], [25] and Power [26], [27].

Translationally periodic bond/node bar-joint frameworks or networks are ubiquitous in mathematics (periodic tilings for example), solid state

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physics (crystal lattices, graphene), solid state chemistry (zeolites) and material science (microporous metal organic frameworks). So there is no lack of interesting examples. I shall illustrate a number of concepts with three examples derived from tilings seen in Seville at the Alcazar and the Cathedral.

2. MODELS FOR MATERIAL CRYSTALS AND LOW ENERGY PHONONS.

We begin by outlining one particular motivation from material science. A crystal framework \mathcal{C} in \mathbb{R}^3 can serve as a mathematical model for the essential geometry of the disposition of atoms and bonds in a material crystal \mathcal{M} . In the model of interest to us the vertices correspond to certain atoms while the edges correspond in some way to strong bonds. Also the identification of strongly bonded "units" in \mathcal{M} imply a polyhedral net structure and it is this that gives the relevant abstract framework \mathcal{C} . A fundamental example of this kind is quartz, SiO_2 , in which each silicon atom lies at the centre of a strongly bonded SiO_4 unit, which in turn may be modeled as a tetrahedron with an oxygen atom at each vertex. In this way the material crystal quartz provides a mathematical crystal framework of pairwise connected tetrahedra with a particular connectedness and geometry.

Material scientists are interested in the manifestation and explanation of various forms of low energy motion and oscillation in materials. Of particular interest are the rigid unit modes in aluminosilicate crystals and zeolites, where quite complicated tetrahedral net models are relevant. These low energy (long wavelength) phonon modes are observed in neutron scattering experiments and have been shown to correlate closely with the modes observed in computational simulations. There is now a considerable body of literature tabulating the (reduced) wave vectors of RUMs of various crystals as subsets of the unit cube (Brillouin zone) and it has become evident that the primary determinant is the geometric structure of the abstract frameworks \mathcal{C} . See, for example, Dove et al [8], Hammond et al [12], [13], Giddy et al [10] and Swainson and Dove [32]. Particularly intriguing is the simulation study in Dove et al [8] which gives a range of pictures of the RUM spectrum and multiplicities for various idealized crystal types.

In the experiments and in the simulations the background mathematical model is classical lattice dynamics and rigid unit modes are observed where the phonon dispersion curves indicate vanishing energy. However, one can also identify such limiting cases through a direct linear approach as we outline below and from this it follows that these sets (at least in simulations) may be viewed as real algebraic varieties. See Theorem 5.4 below, [25], [26] and Wegner [34]. It is convenient to define the RUM dimension to be the dimension of this algebraic variety. (See Section 5.) In 3D it takes the values 0, 1, 2, 3.

3. AN ILLUSTRATIVE EXAMPLE

The following simple example will serve well to illustrate the notation scheme for general crystal frameworks in d dimensions that we adopt. The example is also of interest in its own right, as we see later.

Figure 1 indicates a translationally periodic bar-joint framework $\mathcal{C} = (G, p)$ determined by a sequence $p = (p_k)$ in \mathbb{R}^2 . The framework edges $[p_i, p_j]$, associated with the edges of the underlying graph G , are viewed as inextensible bars connected at the framework vertices p_k but otherwise unconstrained.

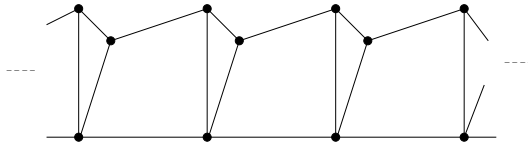


FIGURE 1. An infinite bar-joint framework.

Let the scaling be such that

$$p_1 = p_{1,0} = (0, 0), \quad p_2 = p_{2,0} = (0, 4), \quad p_3 = p_{3,0} = (1, 3)$$

are three framework vertices of a triangular subframework. Write their translates as

$$p_{\kappa,k} = T_k p_{\kappa,0}, \quad \text{for } \kappa \in \{1, 2, 3\}, k \in \mathbb{Z},$$

where T_k is the isometry $T_k : (x, y) \rightarrow (x + 4k, y)$ on \mathbb{R}^2 . The translation group $\mathcal{T} = \{T_k : k \in \mathbb{Z}\}$ is also used to define a natural periodic labelling of the framework edges:

$$e_1 = e_{1,0} = [p_1, p_2], \quad e_2 = e_{2,0} = [p_2, p_3], \quad e_3 = e_{3,0} = [p_1, p_3],$$

$$e_4 = e_{4,0} = [p_{1,0}, p_{1,1}], \quad e_5 = e_{5,0} = [p_{3,0}, p_{2,1}]$$

and

$$e_{j,k} = T_k e_j, \quad \text{for } j \in \{1, 2, 3, 4, 5\}, k \in \mathbb{Z}.$$

Thus, the pair of finite sets

$$F_v = \{p_1, p_2, p_3\}, \quad F_e = \{e_1, \dots, e_5\}$$

have disjoint translates under \mathcal{T} and the set of all such translates determines \mathcal{C} .

In an exactly similar way a translationally periodic bar-joint framework \mathcal{C} in \mathbb{R}^d is determined by a triple (F_v, F_e, \mathcal{T}) where we refer to the finite set pair $\mathcal{M} = (F_v, F_e)$ as a *motif* for \mathcal{C} . Of particular interest for applications are the cases $d = 2, 3$ in which $\mathcal{T} = \{T_k : k \in \mathbb{Z}^d\}$ and \mathcal{T} has full rank. For $d = 3$ "full rank" means that the so-called *period vectors*

$$a_1 = T_{(1,0,0)}(0), \quad a_2 = T_{(0,1,0)}(0), \quad a_3 = T_{(0,0,1)}(0)$$

are linearly independent, in which case the framework vertices, if they are distinct, form a discrete set in \mathbb{R}^3 . We call such discrete bar-joint frameworks *crystal frameworks*.

We now introduce a key dynamical ingredient, namely the notion of an *infinitesimal flex*. This definition is the same as that for finite bar-joint frameworks being a specification of velocity vectors at the nodes which, to first order, do not change edge lengths.

Definition 3.1. Let \mathcal{C} be crystal framework, with framework vertices $p_{\kappa,k}$ as above. An infinitesimal flex of \mathcal{C} is a set of vectors $u_{\kappa,k}$ (velocity vectors) such that for each edge $e = [p_{\kappa,k}, p_{\tau,l}]$

$$\langle p_{\kappa,k} - p_{\tau,l}, u_{\kappa,k} - u_{\tau,l} \rangle = 0.$$

The linear equations required for an infinitesimal flex $u = (u_{\kappa,k})$ translate to a single equation $R(\mathcal{C})u = 0$ where $R(\mathcal{C})$ is the so called *rigidity matrix* for the framework and where u is a vector in the direct product vector space $\mathcal{H}_v = \prod_{\kappa,k} \mathbb{R}^d$, regarded as a composite vector of instantaneous velocities. The rigidity matrix is sparse with rows labelled by edges and columns labelled by the Euclidean coordinate labels (κ, k, σ) of the framework vertices, with $\sigma \in \{1, \dots, d\}$; the row for framework edge $e = [p_i, p_j]$ has the entry $(p_{\kappa,k} - p_{\tau,l})_\sigma$ for column (κ, k, σ) , and has the negative of this entry for column (τ, l, σ) . Thus for $d = 3$ row e appears as

$$[0 \dots 0 \ v_e \ 0 \dots 0 \ -v_e \ 0 \dots 0]$$

where the vector $v_e = p_{\kappa,k} - p_{\tau,l}$ (resp. $-v_e$) is distributed in the columns for (κ, k, σ) (resp. (τ, l, σ)) with $\sigma \in \{x, y, z\}$.

From various viewpoints, such as phase-periodic velocity vectors on the one hand, or square-summable velocity vectors on the other hand, with the introduction of complex scalars and functional representations of vector spaces, the rigidity matrix $R(\mathcal{C})$ leads to a matrix-valued function $\Phi(z)$ with $|F_e|$ rows and $d|F_e|$ columns. The entries are scalar-valued functions on the d -torus of points $z = (z_1, \dots, z_d)$ in \mathbb{C}^d with $|z_i| = 1$.

We define this matrix function below in Definition 5.3 and one can check that the strip framework of Figure 1 has associated matrix function

$$\Phi(z) = \begin{bmatrix} 0 & -4 & 0 & 4 & 0 & 0 \\ 0 & 0 & -1 & 1 & 1 & -1 \\ -1 & -3 & 0 & 0 & 1 & 3 \\ -4(1 - \bar{z}) & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 3\bar{z} & \bar{z} & -3 & -1 \end{bmatrix}.$$

3.1. Examples from Seville. The next three frameworks are based on some simple two-dimensional tessellations that are suggested by tilings found in Seville cathedral (Figures 2 and 3) and in the Alcazar in Seville (Figure 4). All three are in Maxwell counting equilibrium

in the sense that the average coordination number (average vertex degree) is 2, matching the degree of freedom of each vertex, while each subframework is not "overconstrained", in the sense that the number of edges does not exceed twice the number of vertices.

A motif for the framework $\mathcal{C}_{\text{sev}_1}$ is shown in Figure 3 together with the period vectors (dotted). The motif edges consist of a square of edges together with two vertical edges whose (equal) lengths fix the geometry up to a global scaling. (The "rigid units" of this framework are the single vertex subframeworks.)

Note that there is an evident (edge-length preserving) continuous flex, or deformation, $p(t) = (p_{\kappa,k}(t))$ of $\mathcal{C}_{\text{sev}_1}$ which is associated with an expansion in the x direction and a matching contraction in the y direction. We remark that in the case of the geometry with all edge lengths equal this deformation passes through the framework composed of congruent rhombs which is reciprocal (in the lattice sense [6]) to the well-known kagome framework, indicated in Section 5.1. From the first instant of the deformation, so to speak, one obtains an infinitesimal flex $u = p'(0)$ which (unlike infinitesimal translation flexes) is unbounded. Less evident are various nontrivial bounded infinitesimal flexes, but we see below that there are plenty of these and that the RUM dimension is 1.

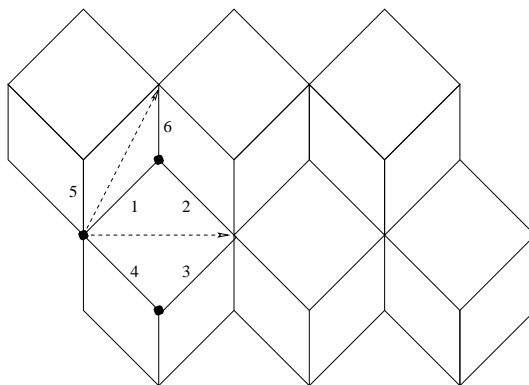
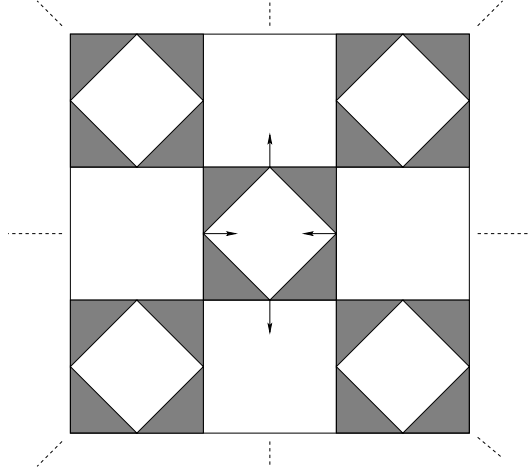


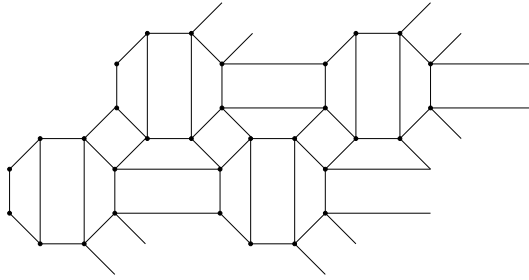
FIGURE 2. The crystal framework $\mathcal{C}_{\text{sev}_1}$.

The framework $\mathcal{C}_{\text{sev}_2}$ in Figure 3 has triangular rigid units and a local (finitely supported) infinitesimal flex is indicated, with four nonzero velocity vector components. It is a general principle, as we note further below, that such a local phenomenon makes the framework maximally flexible from a RUM point of view.

The planar graph, or "topology" of this framework is rather interesting, being a network of 4-rings of triangles connected "square-wise", so

FIGURE 3. $\mathcal{C}_{\text{sev}_2}$, with a local infinitesimal flex.

that the "holes" are 8-cycles and 4-cycles. One can make similar constructions with equilateral triangles with this topology although now the local infinitesimal flex is lost. We remark that periodic networks of pairwise corner-joined congruent equilateral triangles provide the 2D variants of the tetrahedral nets associated with zeolites. (That the hole cycles of 2D zeolites can be arbitrarily large follows from the substitution move which replaces each rigid unit triangle by a 3-ring of smaller triangles with edge length halved.)

FIGURE 4. Part of $\mathcal{C}_{\text{sev}_3}$, a homeomorph of $\mathcal{C}_{\mathbb{Z}^2}$.

The framework $\mathcal{C}_{\text{sev}_3}$ is derived from a tiling in the Alcazar in Seville. A moment's thought reveals it to have the same topology (underlying graph) as that for the basic square grid framework $\mathcal{C}_{\mathbb{Z}^2}$. The infinitesimal flexibility is less evident than is the case for $\mathcal{C}_{\mathbb{Z}^2}$ but from the RUM viewpoint they turn out to be equally flexible with RUM dimension 1.

4. BAR-JOINT FRAMEWORKS - A VERY BRIEF OVERVIEW.

4.1. **Watt, Peaucellier, Cauchy, Euler, Kempe, Maxwell, Laman.**

Informally, a "linkage" is a bar-joint framework with one degree of essential flexibility. In 1784 James Watt designed a bar-joint linkage which transformed circular motion into approximate linear motion. This was rather important for steam engine transmission. The mechanism was approximate and was superseded by Peaucellier's exact linear motion linkage eighty years later. In 1876 Kempe [19] solved the general inverse problem by showing that any finite algebraic curve can be simulated by a linkage. The rigidity of geometric frameworks was also of interest to Euler and to Cauchy who in particular were concerned with the rigidity of polyhedra with hinged faces; a beautiful classical result is the infinitesimal rigidity of all convex triangle-faced polyhedra.

James Clerk Maxwell initiated combinatorial aspects with the observation that a graph $G = (V, E)$ with a minimally rigid generic framework realisation in the plane must satisfy the simple counting rule $2|V| - |E| = 3$ together with the inequalities $2|V'| - |E'| \geq 3$ for all subgraphs. The number 3 represents the number of independent global infinitesimal motions for the plane. In 1970 Laman [20] obtained the fundamental result that Maxwell's conditions are sufficient for generic rigidity and this result also anticipated the advent of matroid theory in rigidity theory. While corresponding counting rules are necessary in three dimensions they fail to be sufficient and no necessary and sufficient combinatorial conditions for generic rigidity are known ! For further information see [1], [2], [11].

4.2. Some Recent work. Laman's theorem concerns *generic* frameworks with a particular graph. One can expect that special frameworks with global symmetries may have more flexibility and this is a topic of current interest. See for example, Connelley et al [5], Owen and Power [23] and Schulze [29], [30]. Understanding constraint systems of geometric objects with symmetry present is also of significance for algorithms for CAD software [23].

Laman's theorem is also concerned with *finite* frameworks. A natural generalisation, also of significance for applications, are periodic frameworks in the sense of the crystal frameworks above. See also Whiteley [33], Borcea and Streinu [4], Malestein and Theran [21], and Ross, Schulze and Whiteley [28].

The theory of general infinite bar-joint frameworks, from the point of view of rigidity, is a novel topic and perhaps a rather curious one. We point out in Owen and Power [24],[22] that it is possible to generalise Kempe's theorem to the effect that any *continuous* curve (ie. continuous image of $[0, 1]$ in \mathbb{R}^2) may be simulated by an infinite linkage. (In [24] this is achieved with three vertices of infinite degree but in fact infinite degree vertices are not necessary.)

In material science the microporous flexing materials known as zeolites are on the one hand important for industrial applications, as filters, and on the other hand present diverse tetrahedral rigid unit frameworks. The degree of continuous flexibility of such idealised zeolites is investigated in Kapko et al [18].

5. THE RUM SPECTRUM AND RUM DIMENSION OF \mathcal{C}

Let $\mathcal{C} = (F_v, F_e, \mathcal{T})$ be a crystal framework in \mathbb{R}^d and let \mathcal{K}_v be the vector space $\prod_{\kappa, k} \mathbb{C}^{|F_v|}$ consisting of infinitesimal velocity vectors. Let \mathbb{T}^d be the d -torus of points $\omega = (\omega_1, \dots, \omega_d)$ and for $k \in \mathbb{Z}^d$ write ω^k for the unimodular complex numbers $\omega_1^{k_1} \dots \omega_d^{k_d}$.

Definition 5.1. ([25], [26].) (a) A velocity vector \tilde{u} in \mathcal{K}_v is periodic-modulo-phase for the (multi-)phase factor $\omega \in \mathbb{T}^d$ if there exists a vector $u = (u_\kappa)$ in $\mathbb{C}^{|F_v|}$ such that

$$\tilde{u}_{\kappa, k} = \omega^k u_\kappa, \quad \kappa \in F_v, k \in \mathbb{Z}^d.$$

Also \mathcal{K}_v^ω denotes the associated vector subspace of such vectors.

(b) A periodic-modulo-phase infinitesimal flex (or wave flex) is a vector \tilde{u} in \mathcal{K}_v^ω which is an infinitesimal flex for \mathcal{C} .

(c) The rigid unit mode spectrum, or RUM spectrum, of \mathcal{C} (with specified translation group \mathcal{T}) is the set $\Omega(\mathcal{C})$ of phases for which there exists a nonzero periodic-modulo-phase infinitesimal flex.

To each multiphase ω there exists a unique wave vector $\mathbf{k} = (\mathbf{k}_1, \dots, \mathbf{k}_d)$ such that $\omega_j = e^{2\pi i \mathbf{k}_j \cdot \mathbf{k}_j}$, $1 \leq j \leq d$. Ignoring bond constraints for the moment, recall that the framework points of \mathcal{C} undergo harmonic motion with wave vector \mathbf{k} when the vertex positions at time t satisfy equations of the form

$$p_{\kappa, k}(t) = p_{\kappa, k} + \exp(2\pi i \mathbf{k} \cdot k) \exp(i\alpha t) v_\kappa,$$

where $\alpha/2\pi$ is the frequency of the oscillation and where $\mathbf{k} \cdot k$ is the inner product $\mathbf{k}_1 \cdot k_1 + \dots + \mathbf{k}_d \cdot k_d$. Such pure motions appear as basic solutions in lattice dynamics, under harmonic approximation, with general solutions obtained by linear superposition. (See Dove [14] for example.)

The following theorem from [26] provides an explanation for the connection between low energy oscillation modes alluded to in Section 2 and infinitesimal wave flexes.

Theorem 5.2. *Let \mathcal{C} be a crystal framework, with specified periodicity, and let \mathbf{k} be a wave vector with point $\omega \in \mathbb{T}^d$. Then the following assertions are equivalent.*

(i) $(\omega^k u_\kappa)_{\kappa, k}$ is a nonzero periodic-modulo-phase infinitesimal (complex) flex for \mathcal{C} .

(ii) For the vertex wave motion

$$p_{\kappa, k}(t) = p_{\kappa, k} + u_\kappa \exp(2\pi i \mathbf{k} \cdot k) \exp(i\alpha t),$$

and a given time interval, $t \in [0, T]$, the bond length changes

$$|p_{\kappa,k}(t) - p_{\tau,l}(t)| - |p_{\kappa,k}(0) - p_{\tau,l}(0)|,$$

for the edges e tend to zero uniformly, in both t and e , as the wavelength $2\pi/\alpha$ tends to infinity.

Next we define the matrix function $\Phi_{\mathcal{C}}$ of a crystal framework \mathcal{C} with given period vectors. For the multi-index $k = (k_1, \dots, k_d)$ write z^k for the usual monomial function on \mathbb{T}^d .

Definition 5.3. Let \mathcal{C} be a crystal framework in \mathbb{R}^d , with motif sets

$$F_v = \{p_{\kappa,0} : 1 \leq \kappa \leq |F_v|\}, \quad F_e = \{e_i : 1 \leq i \leq |F_e|\},$$

and for each edge $e = [p_{\kappa,k}, p_{\tau,l}]$ in F_e let v_e be the edge vector $p_{\kappa,k} - p_{\tau,l}$. The matrix-valued function $\Phi_{\mathcal{C}}(z)$ has rows labelled by the edges $e \in F_e$ and has $d|F_v|$ columns labelled by κ and the coordinate index $\sigma \in \{1, \dots, d\}$. If $\kappa \neq \tau$ for edge e in F_e then

$$(\Phi_{\mathcal{C}}(z))_{e,(\kappa,\sigma)} = (v_e)_{\sigma} \bar{z}^k,$$

$$(\Phi_{\mathcal{C}}(z))_{e,(\tau,\sigma)} = -(v_e)_{\sigma} \bar{z}^l,$$

while for each reflexive edge $[p_{\kappa,0}, p_{\kappa,\delta(e)}]$

$$(\Phi_{\mathcal{C}}(z))_{e,(\kappa,\sigma)} = (v_e)_{\sigma} (1 - \bar{z}^{\delta(e)}),$$

with the remaining entries in each row equal to zero.

The next theorem gives one connection between $\Phi_{\mathcal{C}}(z)$ and the infinitesimal flex properties of \mathcal{C} . Here we view the rigidity matrix $R(\mathcal{C})$ as a linear transformation from the product vector space $\mathcal{K}_v = \prod_{\kappa,k} \mathbb{C}^d$ to the edge vector space $\mathcal{K}_e = \prod_{\text{edges}} \mathbb{C} = \prod_{e,k} \mathbb{C}$.

Theorem 5.4. *The restriction of the rigidity matrix $R(\mathcal{C})$ to the finite dimensional vector space \mathcal{K}_v^{ω} has representing matrix $\Phi_{\mathcal{C}}(\bar{\omega})$ with respect to natural vector space bases.*

Proof. Let \tilde{u} be a velocity vector in \mathcal{K}_v^{ω} determined by $u \in \mathbb{C}^{d|F_v|}$ as above. Let e in F_e be an edge of the form $[p_{\kappa,k}, p_{\tau,k+\delta}]$. Let $\langle \cdot, \cdot \rangle$ denote the bilinear form on \mathbb{C}^d . The $(e, k)^{th}$ entry of $R(\mathcal{C})\tilde{u}$ can be written as

$$\begin{aligned} (R(\mathcal{C})\tilde{u})_{e,k} &= \langle v_e, \tilde{u}_{\kappa,k} \rangle - \langle v_e, \tilde{u}_{\tau,k+\delta} \rangle \\ &= \langle v_e, \omega^k u_{\kappa} \rangle - \langle v_e, \omega^{k+\delta} u_{\tau} \rangle \\ &= \omega^k (\langle v_e, u_{\kappa} \rangle + \langle -\omega^{\delta} v_e, u_{\tau} \rangle), \end{aligned}$$

and one can check that this agrees with $\omega^k(\Phi_{\mathcal{C}}(\bar{\omega})u)_e$, both in the case $\kappa \neq \tau$ and when $\kappa = \tau$. \square

We can now identify the *RUM spectrum* of \mathcal{C} as the algebraic variety in \mathbb{T}^d given by

$$\Omega(\mathcal{C}) = \{z : \text{rank } \Phi_{\mathcal{C}}(z) < |F_e|\}.$$

This set does depend on the choice of translation group. One could define the *primitive RUM spectrum* to correspond to the translation

group for a primitive unit cell, and this is then well-defined, up to coordinate permutations. If one doubles the period vectors, and hence the unit cell, then the new spectrum is obtained simply as the range of the old spectrum under the doubling map $(w_1, w_2, w_3) \rightarrow (w_1^2, w_2^2, w_3^2)$.

While we have given the multiphase form of the RUM spectrum the convention in material science is to indicate such a spectrum (in three dimensions) as the set of (reduced) wave vectors \mathbf{k} in the unit cube $[0, 1)^3$. For calculations of RUM spectrum by different methods see Dove et al [8] (simulation calculations), Wegner [34] (computer algebra calculations), Owen and Power [25] and Power [26] (direct calculations).

The algebraic variety perspective of RUMs appears to be new and opens the way for new methods and terminology for understanding the curious curved surfaces in [8]. For example, it is natural to define the *RUM dimension* of \mathcal{C} to be the topological dimension of $\Omega(\mathcal{C})$ as a real algebraic variety. By the comments above on unit cell doubling it follows that this quantity is independent of the translation group.

Tetrahedral net frameworks in 3 dimensions, with pairwise vertex connection, satisfy Maxwell counting equilibrium and in the periodic case, with no penetrating tetrahedra, are sometimes referred to as hypothetical zeolites [9]. (In material crystalline zeolites the rigidly bonded SiO_4 units make up such a bond-node framework.) Even in this case all possibilities occur for the RUM dimension, namely 0, 1, 2, 3, and this depends, roughly speaking, on the degree of symmetry of the framework. In particular as we note below the framework for the cubic form of sodalite indicated below has full RUM spectrum, corresponding to dimension 3. (This so-called order N property of sodalite was first observed experimentally. See [12].)

For crystal frameworks in Maxwell counting equilibrium the matrix function is square and the RUM spectrum is revealed, in theory at least, as the intersection of the zero set of the multi-variable polynomial $\det \Phi_{\mathcal{C}}(z)$ with the d -torus \mathbb{T}^d . In fact, after fixing a monomial order on the d indeterminates z_1, \dots, z_d one may formally define the *crystal polynomial* $p_{\mathcal{C}}(z)$, associated with \mathcal{C} . (See [26].) This is given as the product $z^{\gamma} \det(\Phi_{\mathcal{C}}(z))$ where the monomial exponent γ is chosen so that

(i) $p_{\mathcal{C}}(z)$ is a linear combination of nonnegative power monomials,

$$p_{\mathcal{C}}(z) = \sum_{\alpha \in \mathbb{Z}_+^d} a_{\alpha} z^{\alpha},$$

(ii) $p_{\mathcal{C}}(z)$ has minimum total degree, and

(iii) $p_{\mathcal{C}}(z)$ has leading monomial with coefficient 1.

The RUM spectrum certainly has symmetry reflecting the crystallographic group symmetries of the crystal framework. Even so the point group may be trivial and the following abstract inverse problem (a Kempe theorem for RUMS ?) may well have an affirmative answer.

Problem. Let $q(z, w)$ be a polynomial with real coefficients with $q(1, 1) = 0$. Is there a crystal framework with crystal polynomial $p(z, w)$ whose zero set on the 2-torus is the same as that for $q(z, w)$?

5.1. Examples. The tiling-derived framework of Figure 3 has vanishing crystal polynomial. Indeed, this can be predicted from the existence of a local infinitesimal flex. Such a flex allows the construction of infinitesimal phase-periodic flexes for all phases and so the zero set of the polynomial includes the entire 2-torus.

The tiling-derived framework of Figure 2 is also in Maxwell counting equilibrium, its symbol function is 6×6 and one can show by direct calculation that if we write the indeterminates in this case as z, w , then the crystal polynomial is

$$(w - 1)(z^2 + z(1 + w) + w)$$

The *kagome framework* is the framework \mathcal{C}_{kag} formed by pairwise corner connected equilateral triangles in regular hexagonal arrangement. Its symbol function is a 6×6 matrix and, if we write the indeterminates in this case as z, w , then the crystal polynomial is

$$(z - 1)(w - 1)(z - w).$$

There is a natural 3D variant of the kagome lattice known as the *kagome net*. The corresponding crystal framework $\mathcal{C}_{\text{knet}}$ has period vectors formed by three edges of a parallelepiped at pairwise angles of $\pi/3$, and each parallelepiped contains two tetrahedral rigid units such that the three planar slices of $\mathcal{C}_{\text{knet}}$ for each pair of period vectors, is a copy of \mathcal{C}_{kag} . The crystal polynomial takes the form

$$p(z, w, u) = (z - 1)(w - 1)(u - 1)(z - w)(w - u)(z - u).$$

The factorisations in these examples makes evident the nature of the RUM spectrum as a union of lines and a union of surfaces, respectively. In fact the individual factors can be predicted in terms of the identification of infinitesimal flexes that are supported within a linear band (for the 2D case) or a linear tube (in the 3D case). See [26]. For considerably more complicated polynomials with nonlinear "exotic" spectrum see Wegner [34] and Power [26].

Figure 4 shows a 4-ring of tetrahedra, three copies of which, placed on three adjacent sides of an imaginary cube, provide the edges and vertices for a motif (F_v, F_e) for the framework \mathcal{C}_{SOD} for the cubic form of sodalite. (From a mathematical perspective, this structure is arguably the most elegant of the naturally occurring zeolite framework types [3].)

A full set of eight 4-rings forms a so-called sodalite cage. With the 24 outer vertices of this cage fixed there is nevertheless an infinitesimal flex of the structure and so a local infinitesimal flex of \mathcal{C}_{SOD} . This is in analogy with the framework $\mathcal{C}_{\text{sev}_2}$. It follows that the determinant

of the symbol function (a 72×72 sparse function matrix) vanishes identically and that the sodalite framework \mathcal{C}_{SOD} has RUM dimension 3.

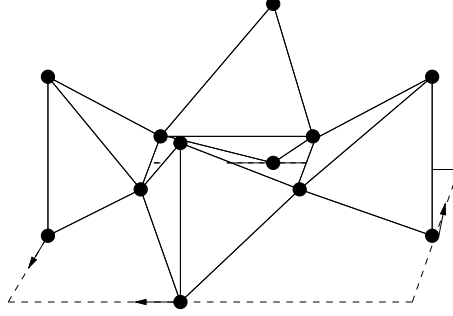


FIGURE 5. A 4-ring building unit from \mathcal{C}_{SOD} .

6. FLEXES WITH DECAY AND TOEPLITZ OPERATORS.

Let \mathcal{C} be a crystal framework with an implicit choice of translational periodicity. Write \mathcal{K}_v^2 and \mathcal{K}_e^2 for the Hilbert spaces of square-summable sequences in \mathcal{K}_v and \mathcal{K}_e . Then $R(\mathcal{C})$ determines a bounded Hilbert space operator from \mathcal{K}_v^2 to \mathcal{K}_e^2 . The natural Hilbert space basis for \mathcal{K}_v^2 , associated with the given periodicity, may be denoted $\{\xi_{\kappa,\sigma,k}\}$, where σ ranges from 1 to d . Similarly, the basis for \mathcal{K}_e^2 is $\{\eta_{e,k}\}$, with $e \in F_e, k \in \mathbb{Z}^d$.

Regarding such square-summable sequences as the Fourier series of square integrable vector-valued functions one obtains unitary operators

$$U_v : \mathcal{K}_v^2 \rightarrow L^2(\mathbb{T}^d) \otimes \mathbb{C}^{|F_v|}$$

and $U_e : \mathcal{K}_e^2 \rightarrow L^2(\mathbb{T}^d) \otimes \mathbb{C}^{|F_e|}$. In the next theorem, from [25], the unitary equivalence referred to is two-sided and the equivalence in question is the operator identity $U_e^* R(\mathcal{C}) U_v = M_{\Phi_{\mathcal{C}}}$. That $U_e^* R(\mathcal{C}) U_v$ has the form of a multiplication operator M_{Ψ} follows from standard operator theory, since this operator intertwines the canonical shift operators. Borrowing standard operator terminology we refer to $\Phi_{\mathcal{C}}$ as the *symbol function* of \mathcal{C} .

Theorem 6.1. *The infinite rigidity matrix $R(\mathcal{C})$ of the crystal framework \mathcal{C} in \mathbb{R}^d determines a Hilbert space operator which is unitarily equivalent to the multiplication operator*

$$M_{\Phi_{\mathcal{C}}} : L^2(\mathbb{T}^d) \otimes \mathbb{C}^{|F_v|} \rightarrow L^2(\mathbb{T}^d) \otimes \mathbb{C}^{|F_e|}.$$

where $\Phi_{\mathcal{C}}$ is the matrix function for \mathcal{C} .

The following corollary follows from elementary operator theory.

Corollary 6.2. *A crystal framework has a square-summable infinitesimal flex if and only if its symbol function has reduced column rank on a set of positive measure.*

It is natural to ask whether crystal frameworks possess infinitesimal flexes which decay to zero at infinity. Note that if an infinitesimal linear subframework has an infinitesimal flex with such decay then the flex velocities must be orthogonal to the direction of this subframework. (For otherwise there must be identical nonzero velocity components in that direction on all the subframework points.) For this reason it follows that the kagome framework and similar "linear" frameworks have no asymptotically vanishing flexes and in particular, no square-summable flexes. In fact one can exploit the matrix function formalism to obtain the following much more general fact.

Theorem 6.3. [25] *The following are equivalent for a crystal framework \mathcal{C} with Maxwell counting equilibrium.*

- (i) \mathcal{C} has a nonzero internal ("finitely-supported", "local") infinitesimal flex
- (ii) \mathcal{C} has a nonzero summable infinitesimal flex.
- (iii) \mathcal{C} has a nonzero square-summable infinitesimal flex.

6.1. Semi-infinite and bi-crystal frameworks. We may define a *semi-infinite crystal framework* \mathcal{D} as a subframework of a crystal framework \mathcal{C} with an exposed face. More formally \mathcal{D} is supported by the framework vertices that lie in a half-space which is invariant under a subsemigroup of an underlying translation group for \mathcal{C} . In the case of planar frameworks this may be specified in the form of a triple $(F_v, F_e, \mathcal{T}_+)$ where (F_v, F_e) is an appropriate motif and \mathcal{T}_+ is a subsemigroup of \mathcal{T} isomorphic to one of $\mathbb{Z}_+ \times \mathbb{Z}$, $\mathbb{Z}_- \times \mathbb{Z}$, $\mathbb{Z} \times \mathbb{Z}_+$, $\mathbb{Z} \times \mathbb{Z}_-$. It is not hard to verify that the rigidity operators of semi-infinite crystal frameworks can be identified with various Toeplitz operators derived from $M_{\Phi_{\mathcal{C}}}$ by compression to Hardy space Hilbert spaces, such as $H^2(\mathbb{T}) \otimes L^2(\mathbb{T})$ in the case of $\mathbb{Z}_+ \times \mathbb{Z}$.

We remark that semi-infinite frameworks have rigidity matrices that feature as block submatrices of the rigidity matrices of *bi-crystal frameworks*. By this we mean (for example) a framework obtained in three dimensions by identifying two semi-infinite frameworks at their common surface of vertices, when this is possible. It seems that Toeplitz operators could provide a useful formalism for their analysis.¹

For semi-infinite crystal frameworks the equivalence of the previous theorem no longer holds and we illustrate this with a simple variant of the strip framework in Figure 1 whose matricial symbol function $\Phi(z)$ is as given in Section 2. Consider the submatrix function $\Phi_0(z)$

¹ Added October 2011. It appears, from [31] for example, that there is extensive interest in material bicrystals.

obtained on removing the first two columns, corresponding to the "supporting" framework vertices, and removing the row corresponding to the "base" edges. The degeneracies of this matrix function correspond to the phases of periodic-modulo-phase infinitesimal flexes which do not deflect the "supporting" vertices. We have

$$\Phi_0(z) = \begin{bmatrix} 0 & 4 & 0 & 0 \\ -1 & 1 & 1 & -1 \\ 0 & 0 & 1 & 3 \\ 3\bar{z} & \bar{z} & -3 & -1 \end{bmatrix}.$$

The determinant, $16(2 - 3\bar{z})$, does not vanish on \mathbb{T} and so the "base-rooted" framework is infinitesimally rigid from the point of view of phase-periodic infinitesimal flexes. Since the determinant certainly does not vanish on a set of positive measure on \mathbb{T} , there are no square-summable infinitesimal flexes which fix the baseline vertices of the framework. On the other hand there is an unbounded infinitesimal flex, corresponding to a two-way infinite geometric series for $z = 2/3$ and this unbounded flex reflects the concatenated lever structure of the framework.

This analysis also applies to the strip framework in Figure 6. One can readily check that up to scalar multiplication there is a unique proper (unbounded) infinitesimal flex. (Note incidentally, that this flex does not extend to a continuous flex. Put another way, each finite strip subframework here is continuously flexible but the complete two-way infinite framework is not. This kind of phenomenon is referred to as *vanishing flexibility* in [25] and can occur in more subtle ways.)

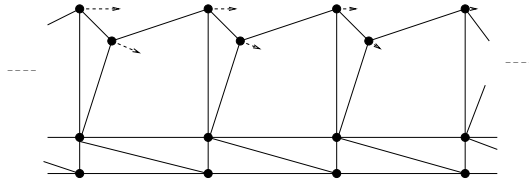


FIGURE 6. An unbounded infinitesimal flex.

There are two natural semi-infinite frameworks $\mathcal{C}_+, \mathcal{C}_-$ associated with the strip framework of Figure 6, namely the right strip and the left strip. Each has a infinite triangulated rigid base framework which supports linked triangles. The former has a square-summable flex while the latter does not. This fact is evident by elementary direct analysis and in fact can be viewed as a reflection of the contrasting nature of analytic and coanalytic Toeplitz operators. We expect such operator theory to play a useful role in the analysis of more complex examples

with larger unit cells, and in the analysis of surface phonons and surface phenomena in semi-infinite structures.

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